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Ranges of Applicability for the Continuum-beam Model in the Constitutive Analysis of Carbon Nanotubes: Nanotubes or Nano-beams?

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RANGES OF APPLICABILITY FOR THE CONTINUUM-BEAM MODEL IN THE CONSTITUTIVE ANALYSIS OF CARBON NANOTUBES: NANOTUBES OR NANO-BEAMS?

VASYL MICHAEL HARIK*

Abstract. Ranges of validity for the continuum-beam model, the length-scale effects and continuum assumptions are analyzed in the framework of scaling analysis of NT structure. Two coupled criteria for the applicability of the continuum model are presented. Scaling analysis of NT buckling and geometric parameters (e.g., diameter and length) is carried out to determine the key non-dimensional parameters that control the buckling strains and modes of NT buckling. A model applicability map, which represents two classes of NTs, is constructed in the space of non-dimensional parameters. In an analogy with continuum mechanics, a mechanical law of geometric similitude is presented for two classes of beam-like NTs having different geometries. Expressions for the critical buckling loads and strains are tailored for the distinct groups of NTs and compared with the data provided by the molecular dynamics simulations. Implications for molecular dynamics simulations and the NT-based scanning probes are discussed.

Key words. nanostructures, nanotubes, mechanical properties, scaling analysis, elasticity

Subject classification. Computational Materials Science

1. Introduction. Carbon nanotubes (NTs) are cylindrical molecules composed of carbon atoms in a periodic hexagonal arrangement. NTs appear to possess extraordinary physical properties such as high stiffness-to-weight and strength-to-weight ratios and enormous electrical and thermal conductivities [1-7]. Potential applications of NTs range from new electronic devices and scanning probes to multifunctional structural components and control systems for aerospace industries. To realize the potential benefits, fundamental understanding of nano-structured material properties and their effect on the associated mechanical behavior is required in order to develop reliable constitutive models for various design purposes.

Recently, the mechanical response of single wall nanotubes (SWNTs) had been evaluated *via* atomistic and molecular dynamics (MD) simulations [1, 2]. In these studies, the structured cylinder models and the continuum Euler beam theory were used to analyze or to deduce the Young's modulus of carbon nanotubes. Yakobson et al. [2] presented a MD simulation of carbon NTs for compressive buckling, and an analogy with macroscopic continuum beams and shells, which had some geometric similarities with NTs and their global behavior, was used. Such analogy provided estimates for the NT Young's modulus, E_{NT}, which may reach as high as 1,000 GPa. Such simple models provide an attractive tool for data reduction and the analysis of structure-property relationships for nano-

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structured materials and carbon NTs, in particular. A macromechanical model *"may serve as a useful guide, but its relevance for a covalent-bonded system of only a few atoms in diameter is far from obvious"* [2]. To ensure the robustness of data reduction schemes that are based on continuum mechanics, a careful analysis of continuum approximations used in macromechanical models and possible limitations of this approach at the nano-scale level is required.

Govindjee and Sackman [6] considered an elastic multi-sheet model of carbon NTs to show the explicit dependence of material properties on the system size when a continuum cross-section assumption is made for a multi-shell system subjected to bending. The continuum assumption was shown to hold when more than 201 shells were present. In the present study, geometric parameters of NT molecular structure are used to define a set of restrictions on a series of assumptions that are used in the Euler beam model. Ru [7] proposed an intrinsic bending stiffness for carbon NTs in order to decouple the bending shell stiffness of NTs from their ill-defined effective thickness and to ensure a consistent use of the classical shell theory [8]. In the current analysis, it is shown the NT thickness may have no direct effect on the buckling behavior of NTs for two classes of molecular structures.

Extensive atomistic and MD simulations of carbon NTs remain computationally expensive and limited in scope. As a result, the continuum models that are appropriately tailored for a particular molecular structure and specific loading conditions may be useful for the qualitative analysis of constitutive behavior of carbon NTs. Since the mechanics of NT response is likely to depend on NT structure, a blend of scaling analysis and continuum mechanics seems appropriate for the development of a methodology for inter-scalar extension of a continuum model to the nano-structures under consideration. This study is focused on beam-like structures and elongated lattice shells that have one dominant dimension as opposed to planar carbon sheets, for instance. Here, to examine possible length-scale limitations of a linear beam model, the underlying continuum assumptions are analyzed in the framework of scaling analysis and hierarchical dimensional analysis of NT buckling and the geometric and material parameters (e.g., the bond length, radius, and elastic modulus).

Dimensional analysis is hardly a verification of physical units, as it may dramatically reduce the number of system parameters by identifying one or two non-dimensional parameters that control the NT buckling behavior. It also helps to select the key ratios that discriminate between different buckling modes and distinct classes of NTs: *short NT shells, long beam-like shells and thin beam-like NTs*. Here, restrictions on the use of a beam model for the last two classes of NTs are derived in the form of applicability criteria and presented along with the model applicability map for different ranges of geometric parameters. Scaling analysis can provide general functional relations for NT buckling response, which indicate the key elements that may appear in formulae for critical buckling loads and strains. The resulting functional relations span the three length scales, which are associated with the size of a carbon ring, the NT radius characterizing the NT cross-sectional size and the length of NTs corresponding to the macromolecular scale. Hierarchical dimensional analysis is also instrumental in deriving a mechanical law of geometric similitude for NT buckling in an analogy with continuum mechanics. Here, the classical buckling formulae are tailored for different classes of NTs and the values of critical strains are compared with the available data for carbon NTs. These formulae embedded into the scaling analysis allow one to consider wide ranges of numerical values for the parameters involved through a few inter-scalar quantities.

The structure of this paper has the following components. First, the problem of nanomechanical buckling is defined along with a description of NT structure, variations of geometric parameters and their effect on geometric properties of NT shells (Section 2.1). An estimate of NT thickness is suggested as well. In Section 2.2, the macromechanical concepts of loading, load transfer and deformation are adjusted to the molecular structure of NTs. Before the continuum beam model is used in Section 3, the aspects of beam-like deformation of NT structures are discussed to illustrate the origin and length-scale limitations of the macroscopic concept of Young's modulus and when it can be applied to carbon NTs. In Section 3.1, two key criteria for the applicability of a linear continuum model are presented. Derivation of the main non-dimensional parameters for NT buckling is carried out in Section 3.2. A mechanical law of geometric similitude is presented in Section 3.3. Ranges of validity for the continuum beam model are summarized in Section 3.4 in a model applicability map and a table. In the discussion (Section 4), unique features of the mechanics of NT buckling are listed along with an overview of classical assumptions of the Euler beam theory. Implications for MD simulations and the design of NT-based scanning probes are also discussed.

2. A nanomechanical problem of NT buckling. Mechanical behavior of molecular structures is likely to depend on the geometric parameters characterizing a particular structural arrangement of atoms and the force fields between them. Here, the continuum model considered neglects all thermal, quantum and electromagnetic effects are neglected. In the problem formulation, the geometry of carbon NTs is defined by a set of parameters and the ranges for their values that characterize the three length scales involved in the buckling problem (Fig. 2). Depending on NT radius and an estimate of NT thickness, the NT shells may be considered either thin or thick. In Section 3, it is shown that both types of geometries are suited for a beam approximation under certain conditions. Here, the loading conditions for the NT molecular structures are also specified along with the type of elastic deformation considered.

2.1. Molecular structure of carbon NTs. Carbon NTs have a lattice-like structure [9] that consists of periodic hexagonal cells of bonded carbon atoms (Fig. 1). The geometric properties of NTs define their structural topology that is similar to beams, for small radii, and cylindrical shells, for large radii. To describe the geometric properties of NTs and their effect on the global behavior of NTs, one has to consider the characteristic parameters that define the NT structural elements, shape, size, etc. In the NT molecules, the smallest dimension is the diameter of carbon atoms (i.e., about 1 Angstrom or 0.1 nm). The adjacent atoms are separated by the distance of about 0.14 nm, that is the length of the C-C bonds or the σ-bond, $l_{c\text{-}c}$. A SWNT consists of many hexagonal carbon rings that have the width, a_1, of about 0.24 nm [5]. The diameter of NTs, d_{NT}, may vary from about 0.4 nm to 100 nm, as a result of various growth conditions (Table 1). The length of NTs, L_{NT}, may also range from about 1 nm to 1 μm or more, depending on the processing conditions. As a result, the NT structure involves three length scales associated with the carbon ring, NT diameter and its length (Fig. 2). A clear separation or collapse of the adjacent length scales results into formation of different classes of NT geometries and structures.

The cross-section of the open molecular lattice of carbon NTs has no continuum thickness, although it has a closed cylindrical structure. The effective thickness of NTs, h_{NT}, can be only estimated. It is bounded by various

estimates between 0.066 nm and the value of interlayer spacing, t, [2, 5]. The interlayer spacing, t, in the multi-wall NTs or layered carbon [5] is relatively large due to the van der Waals forces and is about 0.34 nm. Different estimates are based on models that may address distinct physical effects. The highest interlayer-thickness estimate [5] reflects the effect of van der Waals forces, which may not always play the main role in a deformation. The lowest shell-based estimate [2] is linked to the shell-like buckling behavior of a NT that has a particular geometry. An equivalent-truss model [10] for the planar carbon sheets offers an estimate of 0.28 nm, which is close to the field-based approximation of 0.34 nm.

TABLE 1.

Ranges of the key geometric parameters for carbon NTs

Parameters	Typical Value	Range of Values
The C-C bond length, $l_{c\text{-}c}$	0.144 nm	0.140 – 0.144 nm
Diameter of SWNTs, d_{NT}	10 nm	0.4 – 100 nm
Length of SWNTs, L_{NT}	100 nm	1 nm – 1 μm
Thickness of a SWNT, h_{NT}	?	0.066 – 0.34 nm

For large radii, a NT shell can be defined as a curved, surface-like structure that possesses two characteristics of a closed surface (i.e., L_{NT} and d_{NT}) that are substantially larger than its maximum thickness. In this case, a NT-shell has some dimensional characteristics of a macro-shell. The NT shells of the ratio, h_{NT}/R_{NT}, such that

$$1/1000 < h_{NT}/R_{NT} < 1/10 \quad \text{(thin shell assumption)} \tag{1a}$$

can be considered thin, as the NT thickness is much smaller than its radius. If $h_{NT}/R_{NT} < 1/1000$, then they represent membranes that have negligible bending resistance as in continuum mechanics. In the case of small radii, the NT thickness may not be negligible as compared to the NT radius. In fact, the elastic shells such that

$$h_{NT}/R_{NT} > 1/10 \quad \text{(thick shell assumption)}, \tag{1b}$$

are no longer thin as far as their cross-section is concerned (Table 2).

TABLE 2.

Classification of carbon NT shells based on the thickness-to-radius ratio, h_{NT}/R_{NT}

Estimates for NT thickness, h_{NT}	Thin shells, R_{NT}	Thick shells, R_{NT}
0.34 nm (based on van der Waals forces [5])	3.4 nm - …	0.2 – 3.4 nm
0.28 nm (based on a truss model [10])	2.8 nm - …	0.2 – 2.8 nm
0.072 nm (a half of the C-C bond length)	0.7 nm - …	0.2 – 0.7 nm
0.066 nm (based on a shell analogy [2])	0.6 nm - …	0.2 – 0.6 nm

Inequalities (1) can be considered as the separation criteria for the lowest two length scales (Fig. 2) represented by the thickness of a carbon ring, h_{NT}, and the NT radius, R_{NT}. These length scales merge when the criterion (1b) holds and a class of thick NTs is formed (Table 2). The thin-shell model [2] is most suited when these length scales

are separated, i.e., the criterion (1a) is satisfied. The influence of the largest scale associated with the NT length is critical for the applicability of a beam model to NT buckling as the loading acts along the NT that is about to deform in a deformation mode dependent on its length.

2.2. Loading and deformation of carbon NTs. In continuum mechanics, the material particles of the thin layer that comprises a deforming shell are contained within a top and a bottom bounding surfaces and the edge faces. The middle surface is often used as the reference surface. All of the surfaces are assumed smooth. Here, NT shells are defined by the smooth surface generated by an extension of the 2D lattice of covalent bonds and intersecting centers of the atoms. This middle surface of the equivalent shell is linked to the equilibrium positions of carbon atoms and the lines of relaxed covalent bonds. For NTs, the deforming material is represented by the discrete atoms and the surrounding electron "clouds" that are concentrated along the C-C bonds. The interlayer spacing, t, provides an upper bound for the "thickness" of carbon NTs and a single carbon sheet. Mechanical loading is transferred between the adjacent atoms *via* highly directional covalent bonds. This open lattice-type structure contributes to the reduction in the effective thickness of carbon NTs. Any considerations of homogenization require a minimum number of NT cells along the NT length before any material averaging can be considered unique, i.e.,

$$L_{NT}/a_1 > 1/10, \tag{2}$$

where a_1 is the width of a carbon ring [5], i.e., the characteristic dimension of the NT periodic structure. In continuum theories, quantities like L_{NT}/a_1 tend to infinity, while in nanomechanics it may be just a large number: $L_{NT}/a_1 >> 1$. The NT length, L_{NT}, is bounded from above by the onset of tube coiling during manufacturing, which is likely to depend on the ratio, $L_c = L_{NT}/d_{NT}$. Even when the homogenization criterion (2) holds, the compressive mechanical load is still introduced by a uniform axial displacement as opposed to macroscopic theories, which involve axial loads or stresses that are associated with the concept of cross-sectional area [6].

From the mechanical viewpoint, the elastic deformation is limited by the extent of allowable straining during a time period, ΔT. For carbon NTs, the process of elastic deformation should be completely reversible from the thermodynamic point of view. The deforming NT should pass through a sequence of the equilibrium states. This sets a time-scale limit for a continuum model applied to the molecular structures that have significant relaxation time, Δt_λ , i.e., $\Delta t_\lambda << \Delta T$. Relaxation of molecules depends on their temperature.

Linear buckling theories for elastic beams and shells describe the deflections that are smaller than the wall thickness and exhibit very small elastic strains. That is the axial strain should be smaller than the estimated thickness, h_{NT}. Since the mechanical loads are transmitted through the force field of highly localized covalent bonds, the inter-atomic interaction during elastic deformation can be approximated by the harmonic force field and all strains should be smaller than one half of the bond length, $l_{c\text{-}c}/2$. One half of the bond length, $l_{c\text{-}c}$, may serve as an estimate[†] for the NT thickness, h_{NT}, associated with the transfer of mechanical loads (Fig. 1). This estimate of the NT thickness is close to the shell-based value [2], but it has somewhat different physical nature.

[†] The NT thickness can be estimated by evaluating the transverse dimension of a symmetric electron "cloud" in a half of the bond transferring the mechanical load (Fig. 1), i.e., approximately a half of the C-C bond length.

This study of NT buckling covers all ranges of geometric parameters shown in Table 1 as opposed to a particular case of NT geometry. The dimensions of NT molecular structure are integrated into the analysis presented by combining the elements of continuum mechanics and scaling analysis. The concepts of classical mechanics are extended across the length scales along with careful consideration of possible limitations and their sensitivity to the variability in NT dimensions.

3. Analysis of carbon NTs with the continuum beam model: applicability criteria, the key parameters and a law of geometric similitude. To examine possible length-scale limitations of the macroscopic Euler beam theory, all underlying continuum-based assumptions must be scrutinized (Appendix). The range of validity of different assumptions may be defined by using geometric parameters of NT molecular structure (Section 3.1). This approach provides a link between the molecular structure of carbon NTs, their mechanical properties and the beam model for NTs. Here, the analysis is restricted to the linear elastic behavior of the equivalent NT shells, although NTs are capable of relatively large elastic deformations that are potentially nonlinear [5]. This requires a general load-displacement relation,

$$P/A_{NT} \propto (L_{NT} - L_{NTo})^n/L^n_{NTo}\,, \tag{3}$$

to be linear with respect to the NT elongation or compression, $L_{NT} - L_{NTo}$, i.e., $n = 1$, where L_{NTo} is the original NT length.

The constant of proportionality in the relation (3) defines the initial value of the elastic modulus, E_{NT}, of a beam having cross-sectional area, A_{NT}, [6, 8]. The applicability of the continuum area concept is limited to a group of the thick NT shells of small radii that are defined by inequality (1b). As the ratio of NT radius of curvature to the size of a representative structural cell, a_1 (i.e., the ratio χ_a, $\chi_a = R_{NT}/a_1$) approaches unity, the closed molecular structures that have large aspect ratios, L_{NT}/d_{NT}, become similar to a nano-beam in their mechanical response (Section 3.2). That is a carbon NT reaches its *nano-beam radius* when $R_{NT}/a_1 \approx 1$. This condition is valid only for NTs with small radii, and it can be violated by a class of larger NTs [2] since the NT buckling is not always affected by the continuum area nor by the problems of thickness estimates [7]. Here, in contrast to other studies [2, 6, 7], both classes of NTs are investigated.

3.1. Criteria for the validity of continuum assumptions. The classical Euler beam theory of continuum mechanics is based on a number of assumptions (Appendix) that provide a rigorous framework for deriving governing equations for the deformation of solid beams and specify possible limitations for the beam theory [8]. For the validity of most assumptions, all elastic strains have to be negligible as compared to the NT axial strain, ε_{11}. It can be approximated by $\varepsilon_{11} \approx (L_{NT} - L_{NTo})/L_{NTo}$, where L_{NTo} is the original NT length. In the lattice-beams [9] that are susceptible to transverse shear, the shear may not be small unless the axial strain is infinitesimal, i.e., the length of a NT remains essentially constant. Such constraints hold if

$$\varepsilon_{11} \approx (L_{NT} - L_{NTo})/L_{NTo} << 1. \tag{4a}$$

Criterion (4a) may be satisfied only by long NTs.

The key geometric assumption, which is not always quantified, and the validity of other assumptions depend on the aspect ratio of carbon NTs (i.e., the ratio of their diameter, d_{NT}, to the length, L_{NT}). An appropriate range of aspect ratios can be defined by the following inequality

$$d_{NT}/L_{NT} < 1/10. \tag{4b}$$

This requirement, which is less restrictive than a condition: $d_{NT}/L_{NT} << 1$, is satisfied by two classes of NTs: *long NT shells and thin beam-like NTs*. It also sets a lower limit for the size of the molecular systems in the MD simulations that use the beam model in data reduction. Moreover, it ensures the separation of molecular length-scales (i.e., $L_{NT}/a_1 >> 1$), which is required for obtaining the effective material properties via averaging or homogenization of NT structure. Criterion (4b) also distinguishes the beam deformation modes from the shell buckling modes for NTs with moderate and large radii. The MD data [2] supports the last conclusion.

Applicability of the continuum beam model that is based on the Euler beam theory is limited to the NTs of high aspect ratios, i.e., inequality (4b) should be satisfied. The compressive axial strains should be small as required by inequality (4a) for linear elastic deformation. Two classes of carbon NTs defined by inequalities (1a) and (1b) may satisfy these requirements (i.e., thin and thick NT shells in Table 2). The value of NT Young's modulus, E_{NT}, however, should not depend on the size of a NT. As a result, the concept of NT Young's modulus, E_{NT}, is most applicable when a carbon NT reaches its *nano-beam radius*, $R_{NT}/a_1 \approx 1$. For large values of NT radius, the continuum assumption about the cross-sectional area of a NT does not hold, and the Young's modulus of NT lattice is more appropriate along with the stiffness parameters for shells [2]. However, the continuum beam model may be utilized to estimate the critical buckling strain of thin high-aspect-ratio shells.

3.2. The key non-dimensional parameters for the buckling of *thick* NT-shells. For carbon NTs of small radii, the Euler beam model (Appendix) may qualitatively describe the process of buckling. In the Appendix, it is noted that the critical load, P_{cr}, for the initiation of buckling deformation mode strongly depends on the end conditions of a NT. The global response of a beam depends on the product of its Young's modulus, E_{NT}, and its moment of inertia, I_{NT}, which also depends on the continuum cross-sectional area, $I_{NT} = A_{NT} R^2_{NT}$. Since the dependence of the NT moment of inertia, I_{NT}, on its radius is explicit, $I_{NT} = \pi R^4_{NT}$, general expressions for the critical load, P_{cr}, stress, σ_{cr}, and strain, ε_{cr}, can be written without it, i.e., their functional dependence on NT parameters is given by

$$\sigma_{cr} = f_1(E_{NT}, L_{NT}, d_{NT}, a_1), \tag{5a}$$

or, after introducing three non-dimensional quantities,

$$\frac{\sigma_{cr}}{E_{NT}} = f_{beam}\left(\frac{\pi R_{NT}{}^2}{L_{NT}{}^2}, \frac{R_{NT}}{a_1}\right), \tag{5b}$$

where f_1 and f_{beam} are real-valued functions in the dimensional analysis of the onset of buckling. Here, parameters L_{NT}, R_{NT}, and a_1 represent the three length scales involved in this nanomechanical problem. Hence, the scaling analysis is carried out with the hierarchical dimensional analysis. The number of independent non-dimensional quantities is determined by the dimensional analysis. It is given by the difference between the number of independent parameters and the number of fundamental physical dimensions (i.e., length, time, force). Relation (5b) shows the groups of parameters that are important and may occur in any formulae for linear or nonlinear buckling. Note that the critical strain, ε_{cr}, and the moment of inertia, I_{NT}, are dependent parameters in the functional relations of the dimensional analysis. An important role of the moment of inertia, I_{NT}, in the mechanics of beams is still reflected by the cross-sectional area in the relation (5b). An explicit form of the relation (5b) for a special case of $f_{beam}(\pi R^2_{NT}/L^2_{NT}, R_{NT}/a_1 \approx 1)$ can be given by modifying the Euler buckling formula:[8]

$$\frac{\sigma_{cr}}{E_{NT}} = \frac{P_{cr}}{E_{NT} A_{NT}} = 4\pi \left(\frac{\pi R^2 NT}{L^2 NT} \right) = \varepsilon_{cr} \, . \tag{5c}$$

Here, the ends of a NT are fixed, i.e., the end layer of atoms is constrained. The critical stress, σ_{cr}, and the critical strain, ε_{cr}, $\varepsilon_{cr} \approx (L_{NT} - L_{NTo})/L_{NTo}$, are proportional to the square of the NT aspect ratio, d_{NT}/L_{NT} or the NT cross-sectional area, πR^2_{NT}, normalized by the NT length, L_{NT}. The form of formula (5c) illustrates that even small variations in the value of NT radius or its length may affect the resulting strains or critical loads. Formula (5c) is valid only when the NT aspect ratio, d_{NT}/L_{NT}, satisfies inequality (4b). The assumption of continuum cross-sectional area, A_{NT}, requires that the ratio $\chi_a = R_{NT}/a_1$ is to be small and close to unity. Note that the ratio L_{NT}/a_1 is large when the condition (4b) holds. As a result, the NTs that satisfy these conditions behave as nano-beams of carbon or other material properties.

Note that the two criteria, (4a) and (4b), for the validity of key beam-model assumptions are coupled. Both criteria involve the length, L_{NT}, of NTs that leads to some coupling effects. Figure 3 shows dependence of the critical buckling strain, ε_{cr}, on the aspect ratio of NTs for different values of NT diameter. NT buckling is described by the formula (5c). Notice that for NTs with diameters: d_{NT} = 1 and 2 0 nm, the critical strain, ε_{cr}, is less than 2% only for high values of length, L_{NT}, where both criteria are met. When $R_{NT}/a_1 \approx 1$, the beam model is perfectly applicable (i.e., all values of the strain, ε_{cr}, are below the maximum linear strain of 2%, say) as the NT has reached the nano-beam radius at R_{NT} = 0.2 nm. Note that the three graphs correspond to distinct classes of NTs (Table 2) on the model applicability map (Section 3.4). The coupling effect requires larger NT lengths for larger NT diameters when the linear beam theory is implemented.

Dimensional analysis provides the key non-dimensional quantities that control the physical phenomenon of NT buckling. It means that

the process of NT buckling should remain the same when the NT length, L_{NT}, and NT radius, R_{NT}, change as long as the non-dimensional quantity, $\pi R^2_{NT}/L^2_{NT}$, determined by the dimensional analysis has the same numerical value.

Similarly to the laws of similitude in the dimensional analysis of problems in continuum mechanics, this constitutes

a mechanical law of geometric similitude for the buckling of NTs with small radii.

3.3. The key non-dimensional parameters for the buckling of *thin* NT-shells. The global response of NT shells, for which the assumption of continuum cross-sectional area, A_{NT}, is not valid due to large values of NT radius, can also be qualitatively described by the beam approximation [2]. Here, dimensional analysis can also be carried out for such NTs as it is shown above, to determine the key non-dimensional ratios that control the buckling behavior. For NT shells, a general functional dependence on NT parameters is given by

$$\varepsilon_{cr} = f_2(C_{NT}, D_{NT}, L_{NT}, R_{NT}, h_{NT}), \tag{6a}$$

or, after introducing non-dimensional quantities,

$$\varepsilon_{cr} = f_{shell}(\frac{D_{NT}}{C_{NT}}, \frac{\pi R_{NT}}{L_{NT}}, \frac{h_{NT}}{R_{NT}}) \tag{6b}$$

where f_2 and f_{shell} are real-valued functions, D_{NT} is the bending stiffness and C_{NT} is the axial stiffness of a NT. Note that the critical strain, ε_{cr}, is more appropriate for NTs with no continuum cross-sectional area. Here, NT thickness, h_{NT}, represents the smallest of the three length scales involved as opposed to the cell size, a_1, in the previous class of NTs. For NT shells, when $h_{NT}/R_{NT} << 1$, an explicit form of the critical strain relation (6b) can be again derived by modifying the corresponding Euler formula:[8]

$$\varepsilon_{cr} = 4\left(\frac{\pi R_{NT}}{L_{NT}}\right)^2 \approx \frac{L_{NT} - L_{NTo}}{L_{NTo}}. \tag{6c}$$

is valid for a special case when $R_{NT}/L_{NT} << 1$, while the condition, $D_{NT}/C_{NT} << 1$, is automatically satisfied. These restrictions and the applicability criteria (4) should be specified, when these or similar formulae for buckling are used [2]. The scaling analysis extends the applicability of formula (6c) for a class of NT shells having various geometric parameters (Table 1). A factor "4" in formula (6c) depends on the boundary conditions (Appendix). Significance of non-dimensional ratios such as h_{NT}/R_{NT}, R_{NT}/L_{NT} or d_{NT}/L_{NT}, $\pi R_{NT}/L_{NT}$, and D_{NT}/C_{NT} is underscored here by the dimensional analysis. Note that the important non-dimensional quantity, $R^2_{NT}/R_{NT}L_{NT}$, describing the ratio of the NT cross-sectional area, A_{NT}, to its lateral surface, $2\pi R_{NT}L_{NT}$, is dependent on the NT aspect ratio, d_{NT}/L_{NT}. The ratio h_{NT}/R_{NT} is critical for NTs of low aspect ratios, i.e. when the criteria (4a) is not met by the NT geometric parameters. The data of MD simulations [2] confirm these conclusions.

The molecular structure of thin NTs is different from that of the "thick" NT shells (Section 3.2). However, there are conditions under which NTs of large radii (or the thin shells in Table 2), may behave as beams. When the formula (6c) is valid under the aforementioned conditions, the critical strains for the onset of NT buckling is shown in Fig. 4 for the cases of relatively large radii. Dependence of the buckling strain, ε_{cr}, on the aspect ratio of NTs is quadratic as in the case of thinner NTs (Fig. 3). However, the coupling of two criteria, (4a) and (4b), through the length, L_{NT}, imposes some restrictions on the range of aspect ratios, d_{NT}/L_{NT}, in order to preserve the validity of

beam-model assumptions. The larger is the NT diameter, the smaller the aspect-ratio value should be. For NTs with diameters: d_{NT} = 5 and 10 nm, the critical strain, ε_{cr}, is less than 2% only for very high values of length, L_{NT}, where both criteria are met.

Note that the correctness of dimensional analysis is illustrated by the fact that the critical values of loads (5c) and strains (6c) for the onset of buckling are expressed only in terms of non-dimensional ratios of geometric parameters without adding additional parameters. Although, the aspect ratio, d_{NT}/L_{NT}, controls the key values in both equations (5c) and (6c), the numerators of both non-dimensional quantities have different physical nature that emphasize the known sensitivity to geometric variations in the cross-sectional area and perimeter for beams and shells, respectively. As a result, a more general form of the mechanical law of geometric similitude stipulates that *NTs and nano-rods with different values of d_{NT} and L_{NT} have identical buckling behavior and strains as long as the aspect ratio, d_{NT}/L_{NT}, remains the same*. This law also holds for non-carbon nano-rods. For short NTs, the key ratio is h_{NT}/R_{NT}. Therefore, this law allows one to reduce the number of MD simulations that are needed to describe a class of NTs or nano-rods.

3.4. A model applicability map. Ranges of applicability for the continuum beam model span two different groups of geometric parameters that define two different classes of NTs with small and large values of radius (Tables 2). It is shown above that NTs may have the same buckling behavior, although other mechanical properties (e.g., transverse stiffness) may diverge due to different structural characteristics [1]. Identification of the key non-dimensional ratios of geometric parameters is important for the ability to apply the classical Euler formula across the length scales for a variety of NT geometries. These non-dimensional quantities may also be used to subdivide NTs into several classes of SWNTs that have distinct mechanical behavior due to different structural characteristics. For example, NTs with the small values of a ratio, χ_l, $\chi_l = R_{NT}/l_{c\text{-}c}$, (1.5, say) have high transverse stiffness due to their tight structure, significant curvature and highly pre-strained and pre-stressed covalent bonds. Such NTs loose thin shell characteristics (Table 2). For large values of the ratio χ_l (100, say), NTs have large diameters, lower curvature and the covalent bonds in the form which is close to or identical to those in a sheet of carbon atoms [4, 5]. Such NTs are prone to inward buckling [1] or even flattening. These structural differences in the SWNTs may lead to different overall mechanical responses that would require different mechanical models. Mechanical behavior of different classes of SWNTs can be characterized by dimensional analysis of the NT buckling and their geometric parameters. Tables 1 and 2 provide a summary of ranges for the NT geometric parameters and classes of NTs considered in this study.

Applicability of the continuum beam model for NT buckling can be described by a model applicability map with two regions having different ranges of geometric parameters (Fig. 5). It shows that the beam model fits best for the parameters along the limiting line corresponding to the *nano-beam radius* and the neighboring band. An extension of that band for larger radii and beyond the value of 1/10 would likely involve some micropolar effects [9] in a beam model or an introduction of a shell model. The NT-shells can be also described by the beam model when their aspect ratios, d_{NT}/L_{NT}, are high (i.e., small numerical values of the ratios) even if their radii are relatively large (Table 3). The two classes of NTs may be replaced by the corresponding groups of non-carbon nano-rods (e.g., Co, Fe) as long as they satisfy the two key applicability criteria (4) for a continuum model. This applicability is limited to the

buckling behavior, of course.

TABLE 3.

Restrictions on non-dimensional parameters for the applicability of the continuum beam model

Thin NT shells	Thick NT shells	Carbon nano-beams
$1/L_c < d_{NT} / L_{NT} < 1/10$	$1/L_c < d_{NT} / L_{NT} < 1/10$	$1/L_c < d_{NT} / L_{NT} < 1/10$
$10 < L_{NT} / a_1 < d_{NT}L_c/a_1$	$10 < L_{NT} / a_1 < d_{NT}L_c/a_1$	$10 < L_{NT} / a_1 < d_{NT}L_c/a_1$
$12 < R_{NT} / a_1$	$0.8 < R_{NT} / a_1 < 12$	$R_{NT} / a_1 \approx 1$
$h_{NT} / R_{NT} < 1/10$	$1/10 < h_{NT} / R_{NT}$	$0.33 < h_{NT} / R_{NT} < 1.7$[‡]
$D_{NT} / C_{NT} << 1$	$D_{NT} / C_{NT} << 1$	$D_{NTbeam} / C_{NTbeam} << 1$

4. Discussion of the analysis results on NT buckling. One of the general results of this study is a methodology for the extension of the continuum models across hierarchy of length scales to various nano-structured materials. This study is focused on the molecular lattices that have either one-dimensional beam-like structures or closed cylindrical shapes of elongated shells as opposed to the two-dimensional carbon sheets considered by Odegard et al. [10]. This methodology is defined by a set of criteria that should be satisfied and the hierarchical dimensional analysis that provides the key parameters and the ranges of their values, which control the phenomenon of NT buckling. Some of the results provide useful guidance for MD simulations (Section 4.3) and the design of NT-based scanning probes (Section 4.4). Unique features of the nano-structural buckling are discussed in the next section.

4.1. Mechanics of carbon NTs. The nanomechanical buckling problem has a few distinctions from its macromechanical counterpart [8]. First, the thermodynamic conditions under which the total energy of a molecular system can be equated with the elastic strain energy are important when a linear elastic model is used (Sections 2 and 3). Second, a homogenization criterion for the averaging of material properties has to be introduced, as the macromechanical assumption about an infinite number of atoms does not hold. Third, validity of the assumptions used in the continuum beam model depends on the characteristics of molecular structure of carbon NTs (Section 3.1). Moreover, the physical stresses and strains depend on the local structure of NTs and the corresponding mathematical expressions involve parameters that describe molecular structure of NTs (Sections 3.2 and 3.3).

The displacement boundary conditions are more appropriate and easier to implement for NTs than the load and traction boundary conditions, as the force-displacement relation (3) and the applicability criteria (4) involve either a change in NT length or the NT length itself. The moment of inertia, I_{NT}, is shown to be a dependent parameter (Section 3.2), which can be excluded from the formulae (5) for critical buckling load that involve only independent parameters. Formulae (5) for the critical buckling load are applicable only to NTs of small radii when the concept of continuum cross-sectional area is valid. The applicability of concepts such as the continuum area and the Young's modulus depend on the NT molecular structure (Section 3). Formulae (6) for the critical buckling strain are valid

[‡] These bounds depend on the estimates for NT thickness, h_{NT} (see Table 2).

only for the high-aspect-ratio thin NT shells (Section 3.3). Applicability of these formulae is restricted by the conditions that depend on the length scales involved (Table 3). This analysis is valid only for the linear range of NT deformations that exclude any plastic effects [11].

For small values of the NT radius, the continuum assumption about the cross-sectional area of the NT beam is best satisfied as the ratio R_{NT}/a_1 is close to unity. Note that the geometry of such NTs approaches a topological anomaly (i.e., a collapse of a tubular structure) as the two smallest length scales merge into one. The concept of Young's modulus, E_{NT}, is also most applicable at this limit, although, its value should not depend on the size of a specimen [6, 8]. The importance of cross-sectional area, A_{NT}, for the understanding of NT behavior can also be illustrated by re-writing relation (3) for the linear elastic limit, $n = 1$, as

$$F = g(R_{NT,} E_{NT})(L_{NT} - L_{NTo})/L_{NTo},$$

where F is the force applied to a NT, function g depends on the NT modulus, E_{NT}, and is proportional to the NT radius, i.e., $g(R_{NT,} E_{NT}) \propto R^2_{NT}$.

Assumptions (B1) and (B4) in the Appendix allow the use of one-dimensional theory for capturing the dominant global response features and in deriving the elastic beam equation. Assumption (B2) restricts the direction of displacement of carbon atoms located near the NT edges and the orientation of a single NT. Note that for the type of loading in the assumptions (B1) and (B2), the work done by the applied load is independent of the path it follows during deformation. Requirement (B3) about the constant cross-sectional area leads to the constant moment of inertia, I_{NT}. It is satisfied in the absence of vibrations and temperature gradients. Note that the existence of continuum cross-section is not required for the analysis of NT buckling, in general (Section 3.3). Carbon NTs have very high axial stiffness that satisfies the condition (B5). Assumption (B6) implies that the beam cross-sections do not deform in their planes and their products of inertia are negligible. It requires all cross-sections remain perpendicular to the original image of the beam reference axis during deformation. To control stresses according to the assumption (B9) is problematic for NTs of small radii. In the initial state of relaxed lattice structures, Halicioglu [4] found that the radial stresses are tensile, while the tangential or circumferential stresses are compressive. These stresses are noticeable for the NT diameters such that $d_{NT} < 1$ nm, however their value is small compared to the NT modulus. These internal stresses diminish as the diameters of NTs increase.

4.2. Hierarchical dimensional analysis. The functional relations (5) and (6) have resulted from the hierarchical dimensional analysis that spans the three length scales associated with the size of a carbon ring and the bond length, the NT radius characterizing the NT cross-sectional size and area and the length of NTs corresponding to the macromolecular scale. This analysis is based on a set of inter-scalar non-dimensional quantities (see Table 3). This study is focused on cases when the length scales are well separated. Equations (5) and (6) provide *structure-property relationships* that link the buckling loads and strains of carbon NTs with geometric characteristics of their molecular structure under certain restrictions.

A unique feature of the dimensional analysis is that it allows one to reduce the number of important parameters that characterize a problem and identify the key non-dimensional ratios of such parameters. For example, the

mechanical response of a beam depends on the product of its Young's modulus, E_{NT}, and its moment of inertia, I_{NT}, which also depends on the area, $I_{NT} = A_{NT} R^2_{NT}$. This is reflected in the governing equation for the deflection of beams (Appendix). In Section 3.2, it is proven that this important parameter is not directly relevant. Moreover, in this analysis, the restrictions are formulated with inequalities that allow one to consider wide ranges of numerical values for the parameters involved (see Table 1). Therefore, such analysis is applicable to NTs having different values of geometric parameters. It also reduces the number of MD simulations that are needed to describe a class of carbon NTs (Section 4.3).

4.3. Guidelines for MD simulations. Yakobson et al. [2] have carried out the MD simulations of NTs having d_{NT} = 1 nm. This NT size belongs to the transitional range between thin and thick NT shells (Table 2). Such NTs satisfy the homogenization criterion (2) that sets a lower limit for the size of the molecular systems in the MD simulations, which use the beam model in data reduction. For NTs with L_{NT} > 10 nm, the tube preserved its circular cross-section as it buckled sideways like a beam and as well as during post-buckling. The critical strain was *close* to that for a beam [2]. For shorter NTs, the buckling behavior was dramatically different. Analysis in Section 3 identifies the critical parameters such as an aspect ratio, d_{NT}/L_{NT}, and the inequality, $d_{NT}/L_{NT} < 1/10$, which control this change in the buckling mode. That critical parameter and the criteria for changes in the NT buckling mode are applicable for other NT geometries as well. This fact extends the value of a single MD simulation to other NT geometries.

The dimensional analysis and equations (5) and (6) suggest that the buckling behavior of NTs having the same values of non-dimensional quantities should be similar even if the numerical values of two geometric parameters are different. Indeed, dimensional analysis of the NT shells having finite diameters and large aspect ratios demonstrates that their buckling behavior shown in Fig. 4 should be similar to that of nano-beams (Fig. 3). Similarly to the macromechanical laws of similitude, a mechanical law of geometric similitude is introduced for the nanomechanics of buckling of NT molecular structures. As a result, a single set of MD simulations for NTs within a class of similar NTs can describe the buckling behavior of other NTs as well, according to the law of similitude (Section 3.3). This law allows one to reduce the number of required MD simulations for a group of NTs.

4.4. Design of NT-based scanning probes. Design of NT-based sensory or scanning probes (e.g., AFM tips) may involve selection of NTs with certain mechanical properties (e.g., beam-like behavior). Analysis of Section 3 outlines the conditions under which a NT molecular structure would have a beam-like response, which is required for the effective NT-based AFM probes. The wide range of geometric parameters considered in Tables 2 and 3 allows for the optimization of such probes. NTs with the smallest diameters (the class of carbon nano-beams in Fig. 5) are the closest to the beams as far as their properties and the structure are concerned. In experiments, the direction of loading may not be easily controlled for such NTs at the nano-scale level as the orientation of a single NT, its bonding to the testing device and the control of testing nano-devices are problematic [5].

Implementation of the nano-beam model in data reduction for the sensory experiments that depend on the state of stress in carbon NTs can be affected by the violation of the "stress-free beam" assumption (B7) discussed in the Appendix. It is known that the Young's modulus, E_{NT}, of beam-like NTs can be evaluated as a second derivative of

the elastic strain energy, $\mathcal{E}_{\text{elastic}}$, with respect to the axial strain [2, 8]. The macroscopic expression for the potential energy can be given in terms of the elastic energy: $\mathcal{E}_{\text{elastic}} = \sigma_{ij}\varepsilon_{ij}/2$. For NTs having small radii, R_{NT}, the stress state would be affected by the NT curvature [4]. This fact limits the applicability of this approach for the data reduction.

Experiments that are sensitive to the Poisson's ratio of carbon NTs may also benefit from the consideration of size effects. The Poisson's ratio of graphite is 0.19, same as from the radius reduction in the MD simulations of Yakobson et al. [2]. However, Halicioglu [4] showed that this value is smaller, for NTs with the radii that less than 0.5 nm, and then it reaches a constant for larger NTs. Since the Poisson's ratio is an intrinsic property of a material, it may also serve as an indicator for the nano-beam behavior. As a result, the model applicability map (Fig. 5) may also indicate the structural parameters that define a distinct carbon material, the carbon nano-beam, which has intrinsic properties different from those of a NT shell.

5. Conclusions. Analysis of validity of continuum beam theory for the constitutive behavior of carbon NTs and other nano-rods of non-carbon materials is presented along with the applicability criteria and a model applicability map for the Euler beam model. In particular, the continuum beam model can be used for the qualitative analysis of carbon NTs when

- the homogenization criterion, $L_{NT}/a_1 > 1/10$,
- the aspect ratio criterion, $d_{NT}/L_{NT} < 1/10$, and
- a criterion for the linearity of strains, $(L_{NT} - L_{NTo})/L_{NTo} << 1$,

are satisfied. These criteria set certain requirements for the MD simulations as well. The coupling between the last two applicability criteria for geometric parameters is examined to show the ranges of allowable aspect ratios for different NT diameters. The key non-dimensional parameters that control the onset of NT buckling and the change in buckling modes are identified by the dimensional analysis of NT buckling and the structural parameters characterizing NT molecules. It is shown that the moment of inertia, I_{NT}, is relevant to NT buckling only indirectly. A set of explicit restrictions on these non-dimensional parameters and the applicability of beam models in the data reduction for MD simulations are presented.

A mechanical law of geometric similitude for NT buckling and its generalization are presented for different molecular structures that have the same aspect ratio, d_{NT}/L_{NT}. A model applicability map for two classes of beam-like NTs is constructed for dissimilar ranges of non-dimensional parameters. The law of similitude and the applicability map provide a guide for the extension of applicability of MD simulations from one NT structure to a broad range of NT geometries. Among various NTs that have drastically different geometric properties, a class of carbon nano-beams is identified at the limit of decreasing NT radii. The design of NT-based scanning probes is discussed. Formulae for the buckling loads and strains are tailored for the two classes of NTs and compared with the data provided by the MD studies.

In the hierarchical dimensional analysis, three length scales are represented (i.e., the carbon ring, NT diameter and its length). Such analysis provides a number of functional relations between the physical parameters, σ_{cr} and ε_{cr}, and the geometric parameters that form fewer non-dimensional quantities. It results in *structure-property relationships* that link the buckling strains and critical loads for carbon NTs with the geometric characteristics of their molecular structure. A methodology for the extension of continuum models across the length scales involved

is developed along with a set of criteria that should be satisfied and the hierarchical dimensional analysis that provides the key parameters and the ranges of their values, which control the phenomenon of NT buckling.

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Appendix: The Euler Beam Problem

The beam equilibrium equations for the deflection, $w(x)$, are given by

$$EI\frac{d^2w}{dx^2}+Pw=0,$$

where E is the Young's modulus, I is the moment of inertia and P is the load [8]. Derivation of this equation is based on the following assumptions

B1) deformation of the beam is linear elastic,

B2) the direction of the applied load remains constant during deformation,

B3) the cross-section of the beam does not vary along its length,

B4) the length, L, is much larger than the radius, R, of the beam,

B5) the axial stiffness of the beam is large compared to the bending stiffness,

B6) all deformations of the column occur in the X-Y plane and all cross-sections of the beam remain planar during deformation,

B7) transverse shear deformations are negligible in the beam,

B8) strains in the column are small, but the rotations of the cross-section may be finite,

B9) all stresses are negligible as compared to the axial and shear stresses that act on each cross-section of the beam and in the X-Y plane.

A general solution of the governing equilibrium equation is

$$w(x) = A \sin kx + B \cos kx + Cx + D$$

where $k^2=P/EI$ and A, B, C, D are constants, those values are determined by the boundary conditions. Typical nontrivial solutions, $P_{cr} = n^2\pi^2EI/L^2$, are available for various beams. Here, n = 1, 2, …; and P_{cr} is the critical or Euler load (for n = 1) for a beam with free ends. For pin-joined beams, the critical load is four times lower. For a beam with the ends fixed, it is four times higher (see Timoshenko and Gere [8]).

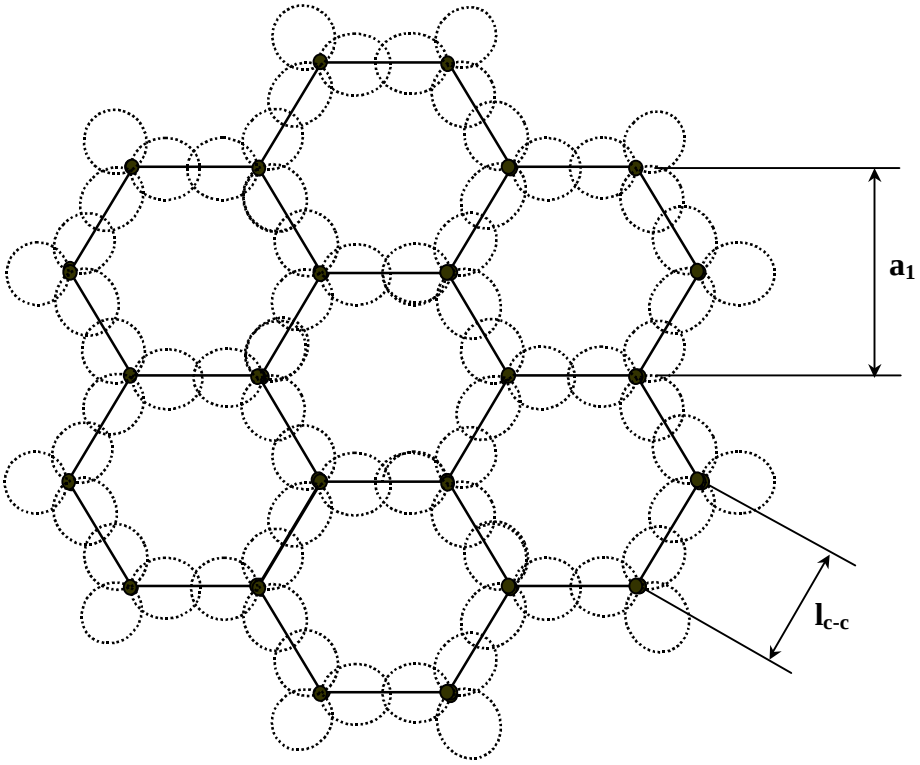

Figure 1. Schematic of a carbon lattice sheet composed of carbon atoms in a periodic hexagonal arrangement. The "thickness" of highly directional covalent bonds, which are formed with electrons from each atom, may approximate the effective thickness of lattice.

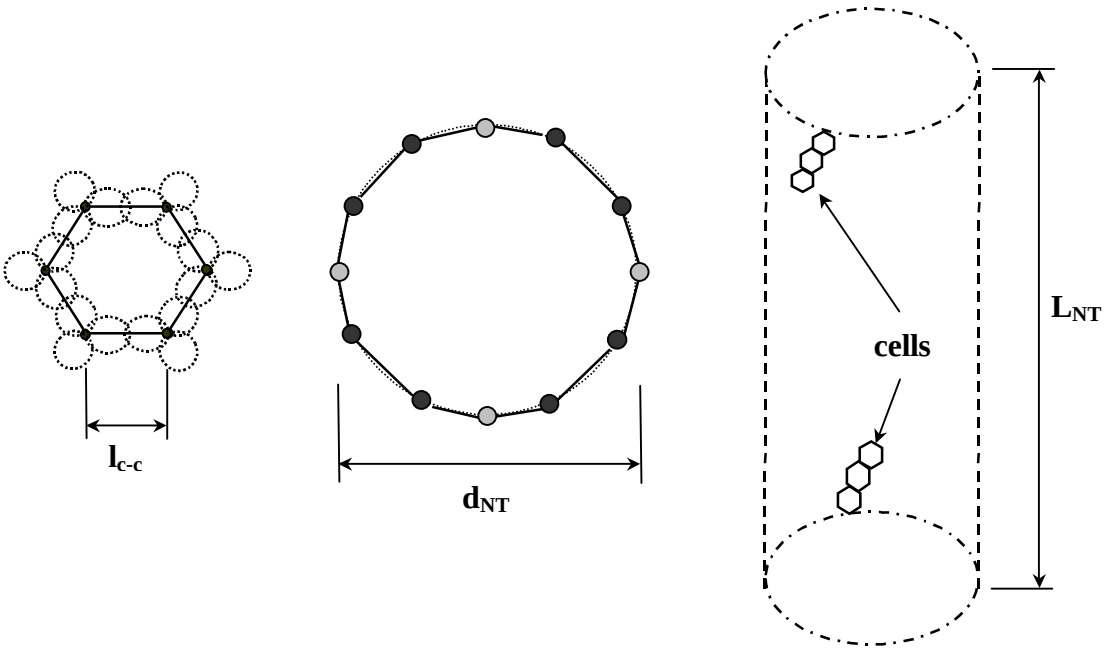

Figure 2. Schematic of a carbon ring, a cross-section of an arm-chair carbon NT and a carbon NT which represent the three length scales involved in the NT buckling problem. Separation and collapse of these length scales result in different classes of NTs.

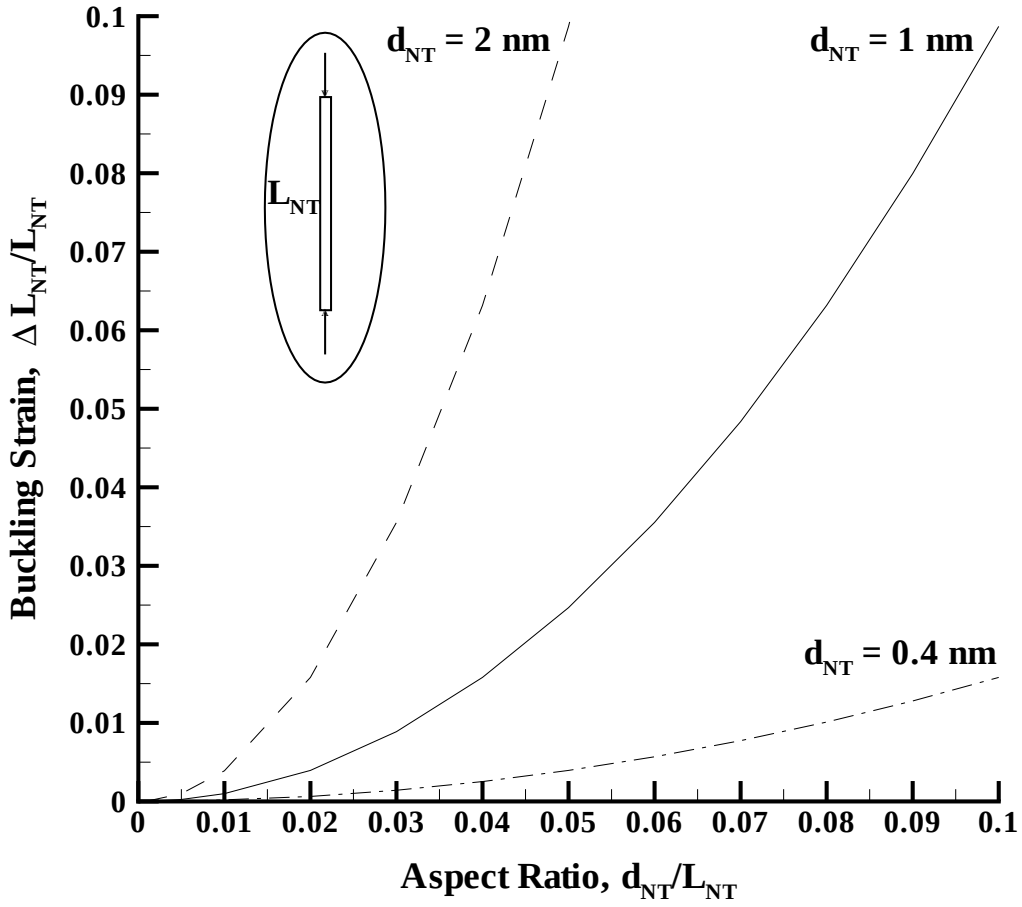

Figure 3. Dependence of the critical buckling strain of carbon NTs on their aspect ratio for various NT diameters. The curve corresponding to the carbon nano-beam limit (d_{NT} = 0.4 nm) lies below the max-strain limit (0.02) for all NT lengths, while other curves require large lengths for the model applicability.

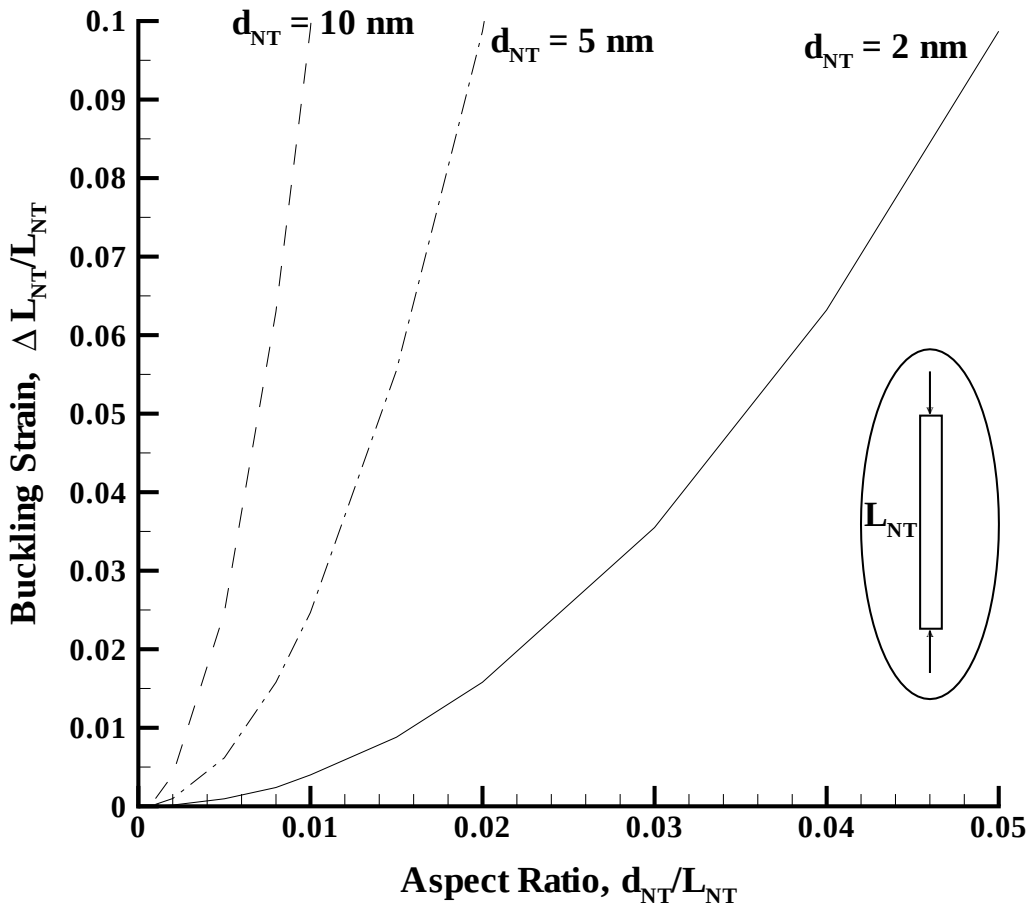

Figure 4. Dependence of the critical buckling strain of carbon NTs on their aspect ratio for relatively large NT diameters. The larger the NT diameter, the larger length of NTs is required for the applicability of the continuum beam model, i.e., the critical strains should stay below the max-strain limit of 2%.

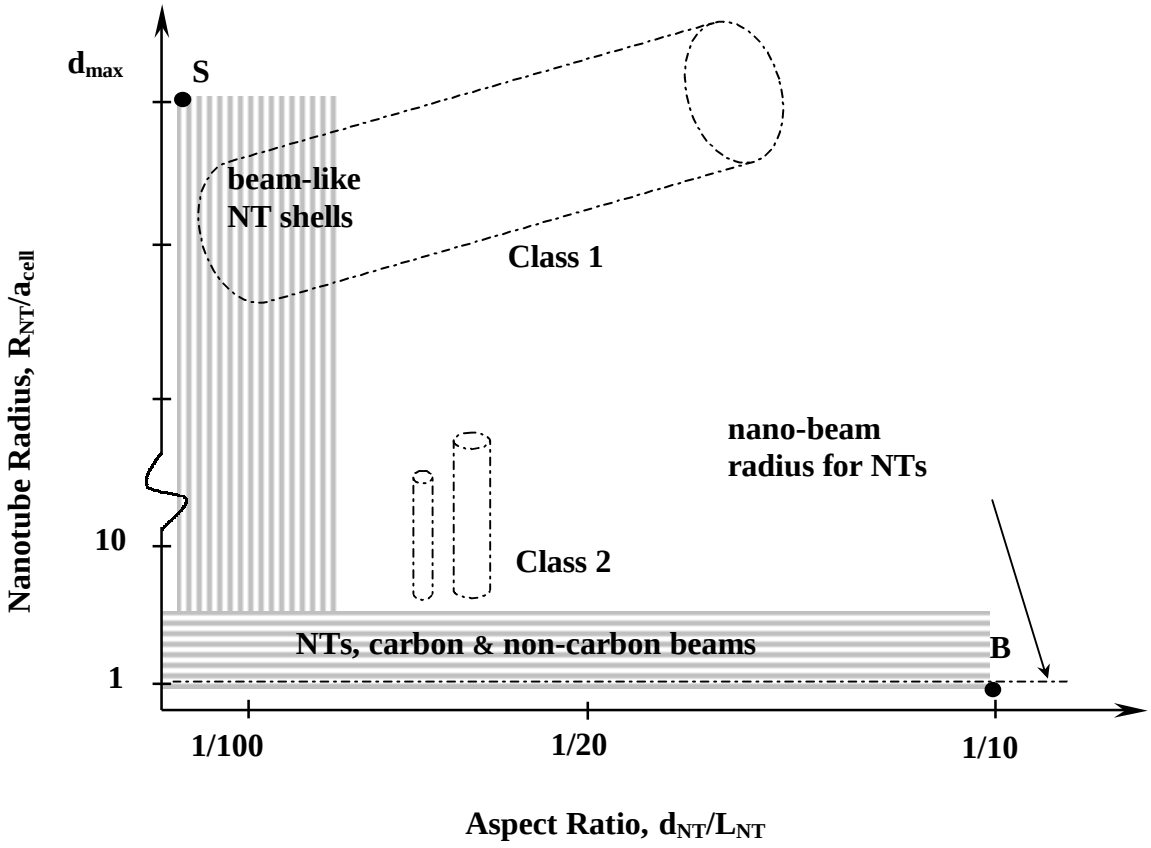

Figure 5. A model applicability map for the continuum beam model depending on non-dimensional ratios of geometric parameters, which are found by the scaling analysis of the constitutive behavior of carbon NTs that belong to two distinct classes of structures and geometries.